# Two Electron Quantum Dot - A Variational Treatment For The Ground State

Subinoy Das
Department of Physics, Indian Institute of Technology, Kanpur, U.P.–208016, India
email: subinoy@iitk.ac.in

Pallab Goswami
Department of Physics, Indian Institute of Technology, Kanpur, U.P.–208016, India
email: pallab@iitk.ac.in

and
J.K. Bhattacharjee[1]
Department of Theoretical Physics, Indian Association for Cultivation of Science
Calcutta – 700032, India
email: tpjkb@mahendra.iacs.res.in

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A variational treatment for a two-electron quantum dot (the artificial helium atom) is proposed which leads to exact answer for the ground state energy. Depending on the magnetic field value the singlet-triplet and triplet-triplet transitions of the ground state take place, which are captured in our solution.Using the same variational technique we find corrections to wave function and energy and the transition field srengths in a realistic dot where electron wave function has a finite extent in the direction perpendicular to the x-y plane in which usually 2-D dot electrons are confined. Using the variational wave function we show that photoemission cross-section as a function of magnetic field has sharp discontinuities, which can be used for experimental verification of the singlet-triplet transitions.

Quantum dots [1] are little two-dimensional islands of electrons, which are laterally confined by an artificial potential. They can be thought of as artificial atoms with the field of nucleus replaced by an imposed external potential.The artificial hydogen atom is a single electron in a two dimensional circular geometry confined by a harmonic potential. The problem becomes interesting in the presence of magnetic field in the perpendicular direction and wave funcions for this case were worked out by Fock [2] shortly after the Schroendiger equation was established. The artificial 'helium atom' problem was, however taken up more than forty years later. In an extensive numerical work Maksym and Chakraborty [3] and Wagner et al [4] found extremely interesting effect of the competition between magnetic field and Coulomb repulsion between electrons in two-electron quantum dots. In particular these authors found that the ground state can change character as the magnetic field changes, leading

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[1]Author to whom all correspondence should be addressed

to singlet-triplet transitions. Six years later Dineykhan and Nazmitdinov [5] using the formidable tools of constructing equivalent hamiltonians in oscillator representations solved the problem for a two-electron quantum dot exactly. In this communication we note the fact that in the real helium atom problem, excellent results for the ground state are obtained by using a variational principle and exploit that to set up a variational calculation for this artificial helium atom. The ground state energy turns out to be the same as obtained from the exact treatment. Employing the same variational techniques we find the required correction for energy, wave function and the magnetic field strengths at which transitions are taking place for a more realistic quantum dot in which elctron wave function has finite extent in the third direction. This is done by imposing a more stronger harmonic confinement in the z-direction. We also show that the photoemission cross-section calculated using the variational wave function has sharp discontinuities at the magnetic field values where the transitions occur which has been proposed to probe it experimentally [6].

For two electrons confined by a parabolic potential in two-dimensional plane,the hamiltonian is (gauge $A_x = \frac{1}{2}By$, $A_y = -\frac{1}{2}Bx$)

$$H = \sum_{j=1}^{2}[-\frac{\hbar^2}{2m^*}\nabla_j^2 + \frac{\omega_c}{2}(-i\hbar\nabla_{\phi_j}) + \frac{1}{2}m^*\Omega^2\rho_j^2] + \frac{e^2}{4\pi\epsilon\epsilon_0}\frac{1}{|\vec{\rho_1} - \vec{\rho_2}|} \tag{1}$$

and if the confinement in the z-direction is considered the hamiltonian is modified by the term

$$H_z = -\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2} + \frac{1}{2}m^*\omega_z^2z^2 \tag{2}$$

and the Coulomb term becomes $\frac{e^2}{4\pi\epsilon\epsilon_0}\frac{1}{|\vec{r_1}-\vec{r_2}|}$. In the $H$ above $\vec{\rho_1}$ and $\vec{\rho_2}$ are the two dimensional position vectors of the two electrons ($\vec{r_1}$ and $\vec{r_2}$ are three dimensional position vectors), $\omega_c = \frac{eB}{m^*}$ is the cyclotron frequency, $\omega_0$ is the frequency of the confining potential in x-y plane ($\omega_z$ is the confining frequency in the z-direction and $\omega_z \gg \omega_0$), $m^*$ is the effective mass of the electron in the semiconductor, $\epsilon$ is the dielectric constant and $\tilde{g}$ is effective Lande factor for the semiconductor and $\Omega^2 = (\omega_0^2 + \frac{\omega_c^2}{4})$. We transform to the center of mass coordinate $\vec{\rho_c} = \frac{1}{2}(\vec{\rho_1} + \vec{\rho_2})$ and the relative coordinate $\vec{\rho_{rel}} = (\vec{\rho_1} - \vec{\rho_2})$ and write the hamiltonian in equation (1) as $H = H_c + H_{rel}$, where $H_{rel} = H_{rel}^0 + H_{int}$ and

$$H_c = -\frac{\hbar^2}{4m^*}\nabla_c^2 + \frac{\omega_c}{2}(-i\hbar\nabla_{\phi_c}) + m^*\Omega^2\rho_c^2 \tag{3}$$

$$H_{rel}^0 = -\frac{\hbar^2}{m^*}\nabla_{rel}^2 + \frac{\omega_c}{2}(-i\hbar\nabla_{\phi_{rel}}) + \frac{1}{4}m^*\Omega^2\rho_{rel}^2 \tag{4}$$

$$H_{int} = \frac{e^2}{4\pi\epsilon\epsilon_0}\frac{1}{\rho_{rel}} \tag{5}$$

The wave function $\Psi(\vec{\rho_c}, \vec{\rho_{rel}})$ will clearly separate as $\psi_1(\vec{\rho_c})\psi_2(\vec{\rho_{rel}})$ with the energy eigenvalue E splitting as $E = E_c + E_{rel}$ where

$$H_c\psi_1(\vec{\rho_c}) = E_c\psi_1(\vec{\rho_c}) \tag{6}$$

$$H_{rel}\psi_2(\vec{\rho_{rel}}) = E_{rel}\psi_2(\vec{\rho_{rel}}) \tag{7}$$

$H_c$ and $H^0_{rel}$ are hamiltonians of single electron quantum dots with the masses of the electrons given by 2m* and m*/2 respectively. Consequently the exact answers are known for these parts and we have

$$
\begin{aligned}
E_c &= (2N+\mid M \mid +1)\hbar\Omega - \frac{\mid M \mid \hbar\omega_c}{2} \\
E^0_{rel} &= (2n+\mid m \mid +1)\hbar\Omega - \frac{\mid m \mid \hbar\omega_c}{2}
\end{aligned}
\tag{8}
$$

with the wave functions given by

$$
\psi_{1NM}(\vec{\rho_c}) = \sqrt{\frac{\Gamma(N+1)}{2^{\mid M \mid +1}\pi \tilde{a}_H^2 \Gamma(N+\mid M \mid +1)}}(\frac{\rho_c}{\tilde{a}_H})^{\mid M \mid}L_N^{\mid m \mid}(\frac{\rho_c^2}{2\tilde{a}_H^2}) \times exp[-\frac{\rho_c^2}{4\tilde{a}_H^2} - iM\phi_c]
\tag{9}
$$

$$
\begin{aligned}
\psi_{2nm}(\vec{\rho_{rel}}) &= \sqrt{\frac{\Gamma(n+1)}{2^{\mid m \mid +1}\pi a_H^2 \Gamma(n+\mid m \mid +1)}}(\frac{\rho_{rel}}{a_H})^{\mid m \mid}L_n^{\mid m \mid}(\frac{\rho_{rel}^2}{2a_H^2}) \times \\
&\quad exp[-\frac{\rho_{rel}^2}{4a_H^2} - im\phi_{rel}]
\end{aligned}
\tag{10}
$$

Here radial quantum numbers N, n are positive integers and angular momentum quantum numbers M, m can take all possible integral values. Length scales are set by $\tilde{a_H}$ and $a_H$ and $\tilde{a}_H^2 = \frac{\hbar}{4m^*\Omega} = \frac{a_H^2}{4}$. In addition to these if we consider the Zeeman term then there would be an energy contribution

$$
E_{spin} = \tilde{g}\mu_B B\sum_{j=1}^{2} S_j^z = \tilde{g}\mu_B B S_{total}^z
\tag{11}
$$

where $S_j^z$ is the z-component of the spin operator of the j-th electron and $\tilde{g}$ is the effective Lande factor for the semiconductor. When permutation of electrons take place $\vec{\rho_{rel}} \rightarrow -\vec{\rho_{rel}}$ and antisymmetry requirement implies for odd m values triplet and for even m values singlet states and $E_{spin} = \tilde{g}\mu_B B(1-(-1)^m)$.

However there is no exact answer for $H_{int}$ and consequently approximation techniques have to be resorted to. Our observation is that the variational principle which one employs to calculate the ground state of helium atom should be effective here as well. This is what prompts our trial wave function. The center of mass motion does not enter the picture, the ground state of that being fixed by $N = M = 0$. In the absence of the Coulomb interaction, the ground state of the relative motion would be given by $n = m = 0$. It is important to note that in the absence of confinement (i.e.$\omega_0 = 0$), the energy levels are independent of m, but in the presence of confining potentials, for a given value of n, there is an interesting dependence on the azimuthal quantum number m. Magnetic field tries to compress the wave function i.e., to decrease the separation of the electrons where as to minimize the Coulomb repulsion electrons would tend to increase their separation. Optimization of these competing effects i.e., minimization of the total energy takes place at different m values depending on the strength of the magnetic field. Now to maintain the anti-symmetry of the total wave function the spin state changes between triplet to singlet corresponding to change in m from odd to even value and vice

versa as evident from the $E_{spin}$ expression. At strong magnetic field due to spin polarization, spin states would be triplets; thus ground state ceases to show further singlet- triplet transition and only triplet-triplet transitions take place. Consequently, in writing down the ground state wave function, we respect this fact by anticipating an n = 0 form for the radial wave function but allowing for an azimuthal dependence as $\exp(-im\phi_{rel})$. As the dominating part of the potential terms in $H_{rel}^0 + H_{int}$ is the parabolic one, the effect of the Coulomb part can be accounted by introducing the length scale as the variational parameter in analogy with the helium atom problem. This inspires the variational trial wave function (normalized)

$$\psi_{0m}(\vec{\rho_{rel}}) = \sqrt{\frac{1}{2^{|m|+1}\pi\beta^2\Gamma(|m|+1)}}(\frac{\rho_{rel}}{\beta})^{|m|}exp[-\frac{\rho_{rel}^2}{4\beta^2} - im\phi_{rel}]$$

(12)

With this trial function, there will be four contributions to $E_{rel}$, which we write as

$$
\begin{aligned}
E_1(\beta, m) &= <\psi_{0m} \mid -\frac{\hbar^2}{m^*}\nabla_{rel}^2 \mid \psi_{0m}> = \frac{\hbar^2}{2m^*\beta^2}(|m|+1) \\
E_2(\beta, m) &= <\psi_{0m} \mid \frac{\omega_c}{2}(-i\hbar\nabla_{\phi_{rel}}) \mid \psi_{0m}> = -\frac{\omega_c m\hbar}{2} \\
E_3(\beta, m) &= <\psi_{0m} \mid \frac{m^*\Omega^2\rho_{rel}^2}{4} \mid \psi_{0m}> = \frac{m^*\Omega^2\beta^2}{2}(|m|+1) \\
E_4(\beta, m) &= <\psi_{0m} \mid \frac{e^2}{4\pi\epsilon_0\epsilon\rho_{rel}} \mid \psi_{0m}> = \frac{e^2\Gamma(|m|+\frac{1}{2})}{4\pi\epsilon_0\epsilon\beta\sqrt{2}\Gamma(|m|+1)}
\end{aligned}
$$

(13)

This leads to

$$E_{rel}(\beta, m) = (|m|+1)[\frac{\hbar^2}{2m^*\beta^2} + \frac{m^*\Omega^2\beta^2}{2}] - \frac{\omega_c m\hbar}{2} + \frac{e^2\Gamma(|m|+\frac{1}{2})}{4\pi\epsilon_0\epsilon\beta\sqrt{2}\Gamma(|m|+1)}$$

(14)

Minimization of this energy with respect to $\beta$ leads to

$$x^4 - \frac{a_H}{a^*}\frac{1}{\sqrt{2}}\frac{\Gamma(|m|+\frac{1}{2})}{\Gamma(|m|+2)}x - 1 = 0$$

(15)

where $x = \frac{\beta}{a_H}$ and $a^* = \frac{4\pi\epsilon_0\epsilon\hbar^2}{m^*e^2}$. We solved equation (15) numerically for GaAs bulk conduction band electron parameters ($g = -0.44$, $\frac{m^*}{m_e} = 0.067$, $\epsilon \approx 13$) and the results are shown in fig.1 and fig.2. We have taken the typical confinement energy to be 4meV and varied B from 0 to 12T. In fig.1 $\frac{E_{rel}+E_{spin}}{\hbar\omega_0}$ vs. B is plotted. The transitions $m = 0 \to m = 1$, $m = 1 \to m = 2$ occur respectively at magnetic field strengths 1.3T, 6.1T (approximately). The mean square separation of two elctrons is given by $<\psi_{0m} \mid \rho_{rel}^2 \mid \psi_{0m}> = 2(|m|+1)\beta^2$ and root mean square separation $d = \frac{\sqrt{<\psi_{0m}|\rho_{rel}^2|\psi_{0m}>}}{a^*}$ vs. B is plotted for different m values in fig.2 showing the discontinuities brought about in the inter-electron separation by the transitions.

However for a more realistic quantum dot the finite extent of the electronic wave function in the third direction has to be taken into account and we achieve this by imposing another harmonic

confinement in the z-direction and employ our variational tools to get the characteristic equation. With the $H_z$ part we have the wavefunction modified by

$$\psi_3(z) = \frac{1}{\sqrt{2^n \Gamma(n_z+1)\pi^{1/2}\lambda}} \exp(-\frac{z^2}{2\lambda^2})H_n(\frac{z}{\lambda}) \tag{16}$$

and the energy is modified by the term $E_z = (n_z+\frac{1}{2})\hbar\omega_z$. Separating the hamiltonian again in center of mass and relative coordinates and following previous arguments it can be clearly seen that the ground state would have quantum numbers $N_z^c = 0$ and $n_z^{rel} = 0$. We introduce the variational parameters $\beta_1$ and $\beta_2$ respectively replacing $a_H$ and $\lambda_{rel}$ and after energy minimization get coupled characteristic equations for $x = \frac{\beta_1}{a_H}$ and $y = \frac{\beta_2}{\lambda_{rel}}$ where $\lambda_{rel}^2 = 2\lambda^2 = \frac{2\hbar}{m^*\omega_z}$. The characteristic equations are

$$x^4[1 - \frac{2}{y^3}(\frac{a_H}{a^*})(\frac{a_H}{\lambda_{rel}})^3 \frac{\Gamma(|m|+1)}{\Gamma(\frac{5}{2}+|m|)} 2F_1(\frac{3}{2}, 2+|m|, \frac{5}{2}+|m|, 1 - 2(\frac{x}{y})^2(\frac{a_H}{\lambda_{rel}})^2)] = 1 \tag{17}$$

$$y^4 - y(\frac{\lambda_{rel}}{a^*})\frac{\Gamma(|m|+1)}{\Gamma(\frac{3}{2}+|m|)} 2F_1(\frac{1}{2}, 1+|m|, \frac{3}{2}+|m|, 1 - 2(\frac{x}{y})^2(\frac{a_H}{\lambda_{rel}})^2) + 2\frac{x^2}{y}\frac{a_H^2}{a^*\lambda_{rel}}\frac{\Gamma(|m|+2)}{\Gamma(\frac{5}{2}+|m|)} \times$$
$$2F_1(\frac{3}{2}, 2+|m|, \frac{5}{2}+|m|, 1 - 2(\frac{x}{y})^2(\frac{a_H}{\lambda_{rel}})^2) = 1 \tag{18}$$

We have solved these coupled equations simultaneously with GaAs parameters and found that singlet-triplet transitions are taking place at higher magnetic field strengths and these results are shown in Fig.3. These results can be understood from the physical ground that with the introduction of harmonic confinement in the z-direction x values decrease significantly compared to the exact 2-D situation (Fig.4) leading to increase in Coulomb energy and to minimize the total energy the required transitions need higher energy contribution from the magnetic field. Therefore, the transitions occur at higher fields strengths. All these results are in good agreement with the exact solution of Dineykhan and Nazmitdinov [5].

Usually the energy levels in the semiconductor quantum dots are probed by the FIR spectroscopy. Due to the long wavelength of the electromagnetic field (compared to the dot size), there is no appreciable change in the electric field across the dot and hence, the elctric field couples only to $H_c$ through the contribution $e\vec{E} \cdot (\vec{\rho_1} + \vec{\rho_2}) \exp(i\omega t) = 2e\vec{E} \cdot \vec{\rho_c} \exp(i\omega t)$, where $\vec{E}$ is a constant electric field (dipole approximation). As $H_{rel}$ is not coupled to the field, FIR spectroscopy does not probe the effects of inter-electron repulsion. However if we consider the photoemission from the dot to the vacuum by irradiating the dot with high energy photons, then $H_{rel}$ is coupled to the external fields (as the wave length is comparable to the dot size, dipole approximation is not valid) and the singlet-triplet and triplet-triplet transitions are manifested as sharp discontinuities in the photoemission cross-section. The calculation of the photoemission cross-section involves the evaluation of a matrix element corresponding to the electromagnetic field operator causing the emission from the initial state to final state and thus depends on the details of the initial and final state wave functions. This dependence

on the initial and final state introduces the m dependence of the cross-section and in this case we do not replace $\exp(i\vec{k} \cdot \vec{r})$ by unity as done in the dipole approximation. The operator is treated exactly and the final form of the differntial cross-section calculated using our analytically found trial wave function becomes

$$\frac{\frac{d\sigma}{d\phi_{\vec{q}}}}{\sigma_0} = \frac{2^{8+3m}}{\Gamma(|m|+1)}[1 - (|m|+1)\frac{\Omega}{\omega} + \frac{m}{2}\frac{\omega_c}{\omega}]\sin^2\theta\cos^2\phi\frac{(x^2+2)^{2|m|}(Ka_H)^{2|m|}}{x^{2|m|-2}(x^2+6)^{2|m|+2}}\exp[-2\frac{K^2a_H^2(3x^2+2)}{(6+x^2)}]$$

$$(19)$$

Here, $\vec{q}$ is the wave vector of the emitted electron, $\vec{k}$ is the wave vector of the incident photon, $\hbar\vec{K} = \hbar(\vec{k} - \vec{q})$ is the momentum transferred and $\theta$ and $\phi$ are respectively the angles $\vec{q}$ makes with $\vec{k}$ and $\vec{k}\hat{n}$ plane where $\hat{n}$ is the unit polarization vector of the incident photon. $\sigma_0 = \frac{e^2}{ca^{*2}}(\frac{m_e}{m^*})^2$ is a constant extracted to express the differntial cross-section expression in a dimensionless form. So,

$$K^2 = k^2 + q^2 - 2kq\cos\theta \qquad (20)$$

holds and $\cos\phi = \sin\theta_{\hat{n}}\cos(\phi_{\hat{n}} - \phi_{\vec{q}})$ and $\cos\theta = \sin\theta_{\vec{k}}\cos(\phi_{\vec{k}} - \phi_{\vec{q}})$. Therefore, it is very clear from the expression for the differential cross-section that it depends significantly on the direction of incidence and polarization. This for some simple cases can be illustrated easily. If $\vec{k}$ is parallel to z-axis then $\cos\theta = 0$ and $\cos\phi = \cos\phi_{\vec{q}}$ or $\cos\phi = \sin\phi_{\vec{q}}$ as $\hat{n}$ is parallel to x or y-axis. So, the angular distribution is proportional to $\cos^2\phi_{\vec{q}}$ or $\sin^2\phi_{\vec{q}}$ and if it is the case of circular polarization then the angular distribution is proportional to $(\cos^2\phi_{\hat{n}}\cos^2\phi_{\vec{q}} + \sin^2\phi_{\hat{n}}\sin^2\phi_{\vec{q}})$ and only if $\hat{n} = \frac{(\hat{x}\pm\hat{y})}{\sqrt{2}}$ then it becomes isotropic. But, when the $\vec{k}$ lies in the x-y plane then with all the cases of circular polarization we shall have angular dependence. It also becomes apparent from the expression that emission count is larger in the direction of polarization compared to other cases and if the photon is linearly polarized in the z-direction then there is no emission. So, depending on the 'm' values of the ground state as a function of magnetic field the cross-section would have different angular distribution as well as discontinuities characterizing transitions of the ground state. Based on these one can probe now these transitions experimentally. In the context of experiment the frequency of the photon has to be carefully chosen as well as those directions mentioned above and details of these shall be provided elsewhere [6] where we also show the modifications in the context of more realistic quantum dots due to finite thickness. For illustration we plot the above expression for the transition $m = 0 \rightarrow m = 1$ and $m = 1 \rightarrow m = 2$ in fig.5.

It should be noted that, using the proper variational wave function for the ground state we have reproduced the exact solution of Dineykhan and Nazmitdinov [5]. The essential features of the interacting two electron ground state of the semiconductor quantum dots, i.e., the singlet-triplet transitions with the change in the magnetic field strength and triplet-triplet transitions at very strong magnetic field are explained using our result. In the triplet state the angular momentum of the ground state is m = 2p + 1,where p is a positive integer and this is weak version of the magic number concept. As, in our choice of the trial wave function the symmetry under permutation is properly taken into

account and the orthonormalization is built in, proceeding in the same way it is quite trivial to find the higher excited states with nonzero radial excitations i.e., $n \neq 0$ . The competing effects of the magnetic field and Coulomb repulsion are also demonstrated in terms of the variational length scale, which captures the discontinuous changes in the inter-electron separation at transition points. Also, by same kind of variational calculation the wave function and energy found for a dot with finite thickness are in good agreement with the physically anticipated results. From the calculated photoemission cross section using the above mentioned trial wave function we have also analytically demonstrated the sharp discontinuities and the difference in the angular distribution at transition points which can be used to probe these transitions for the parabolic dot in addition to the found discontinuities from the magnetization measurement.

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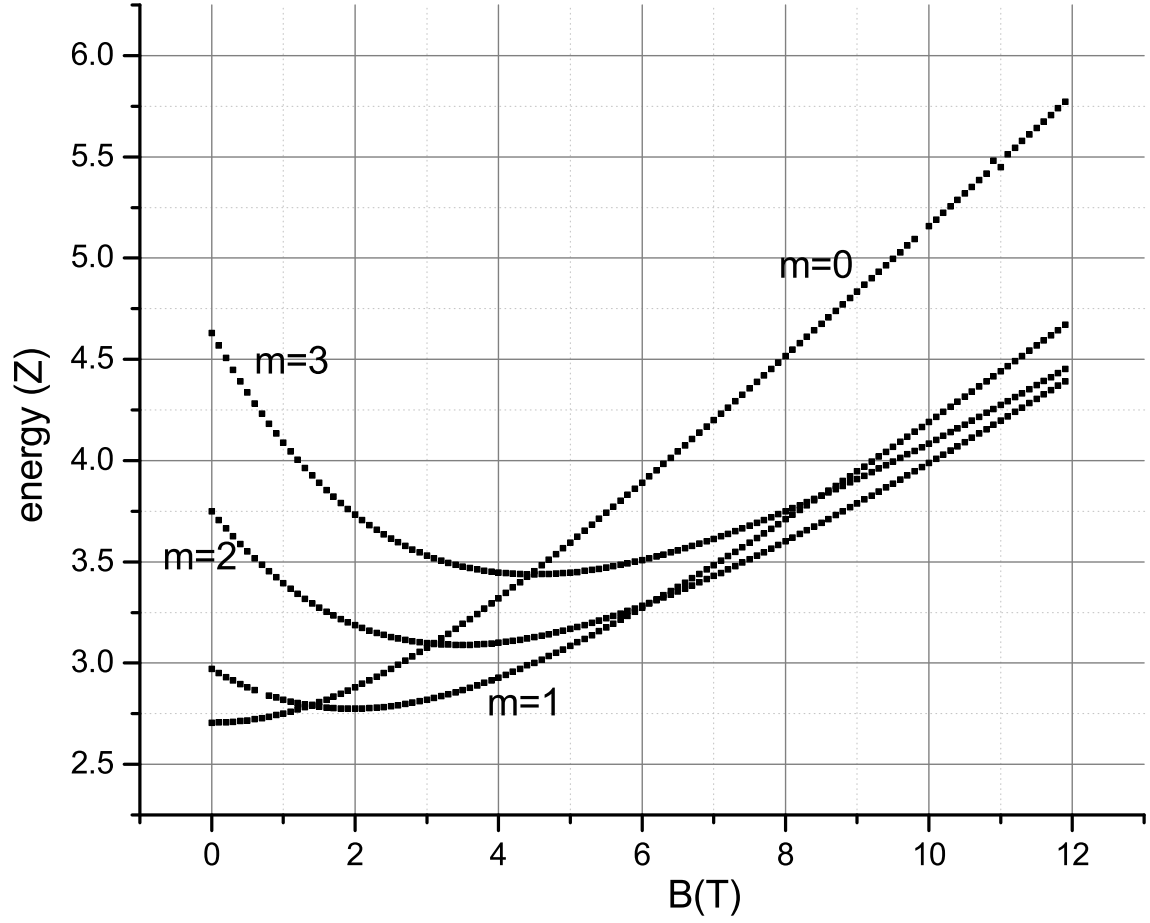
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Figure 1: $Z = \frac{E_{rel} + E_{spin}}{\hbar \omega_0}$ vs. B(T) is plotted for different 'm' values and $m = 0 \rightarrow m = 1$, $m = 1 \rightarrow m = 2$ transitions are taking place at $B = 1.3T$ and $B = 6.1T$ respectively and also other energy level crossings are present.
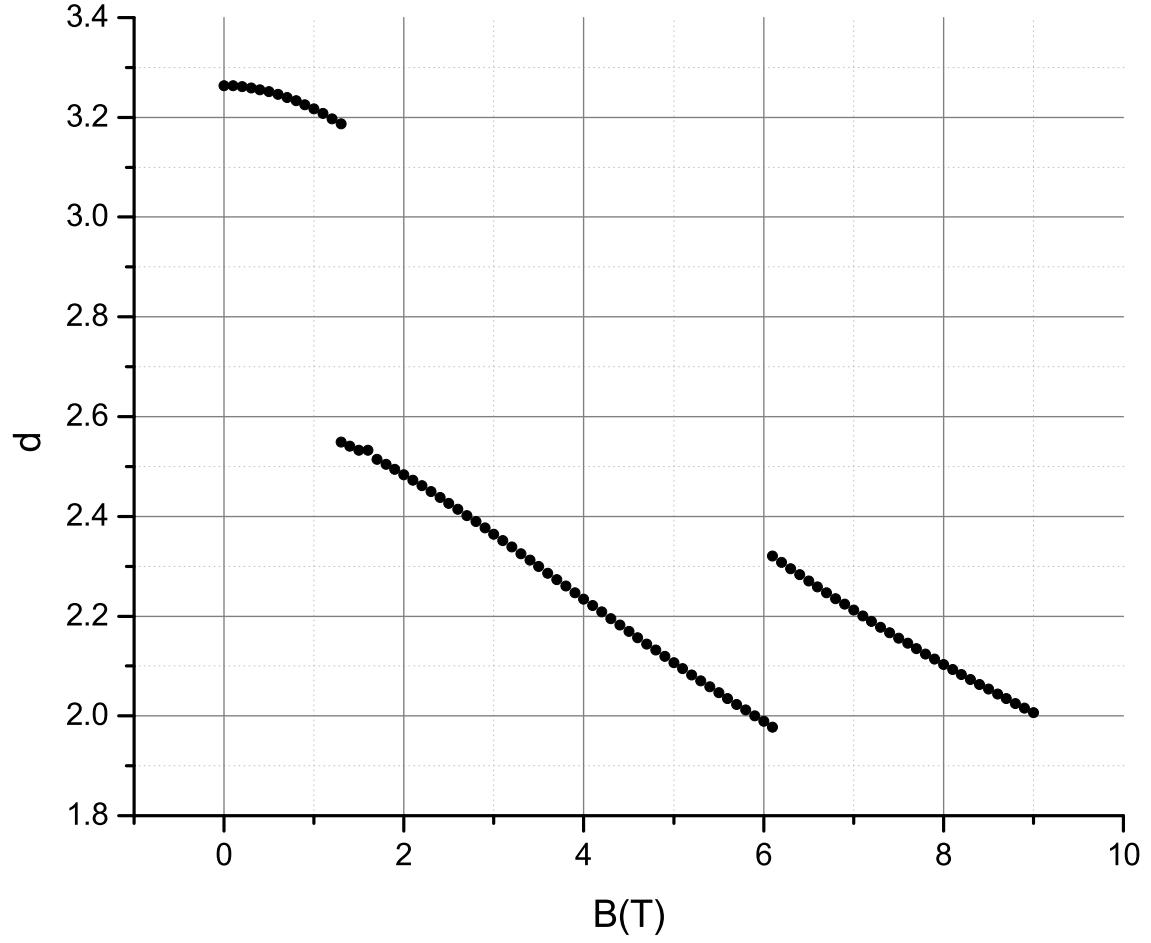
Figure 2: $d = \frac{\sqrt{<\psi_{0m}|\rho^2_{rel}|\psi_{0m}>}}{a^*}$ vs. B(T) is plotted for differnt 'm' values of the ground state and the transitions are captured in the discontinuous changes of d
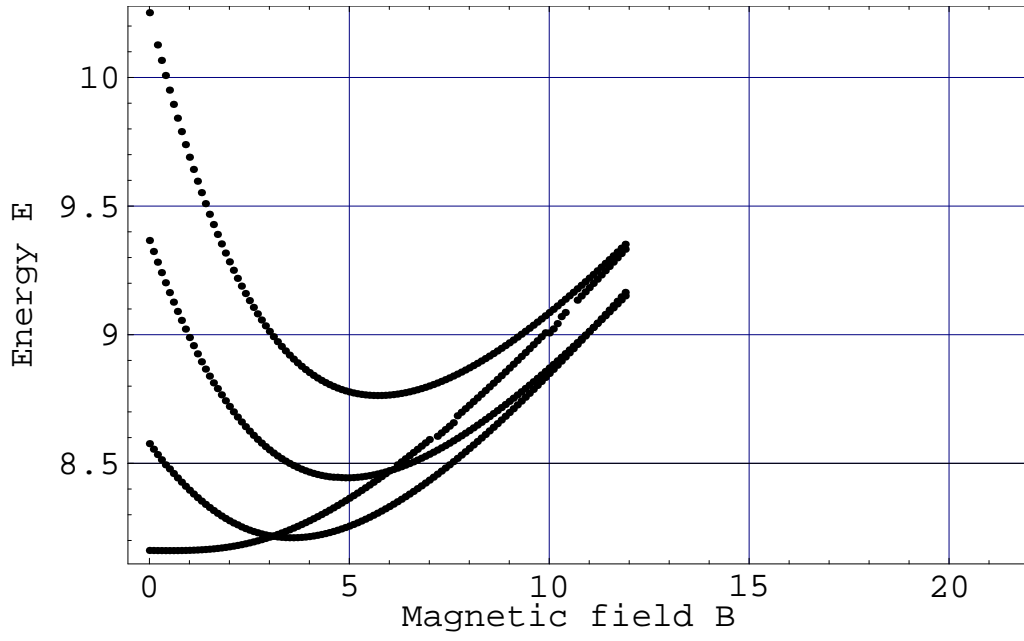
Figure 3: $E = \frac{E_{rel} + E_{spin}}{\hbar\omega_0}$ vs. B(T) plotted for different 'm' values when finite thickness of the dot is taken into account.For this purpose $\frac{\omega_z}{\omega_0} = 9$ has been taken.
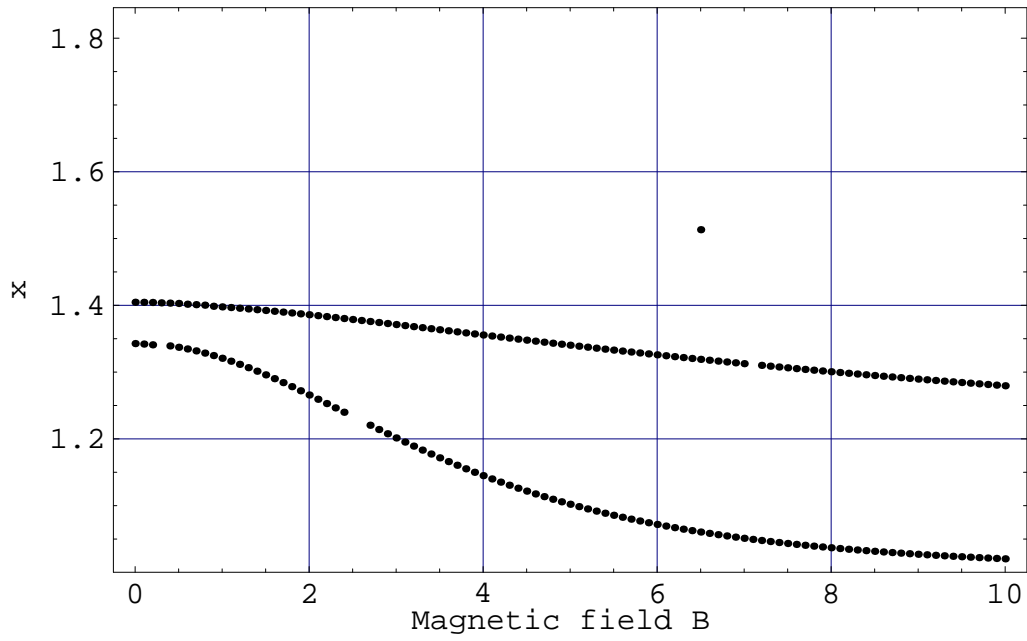
Figure 4: $x$ vs. B(T) is plotted for $m = 0$ for both the 2-D and realistic 3-D dot and it is clearly found that throughout the range of magnetic field x values have decreased for the later one.
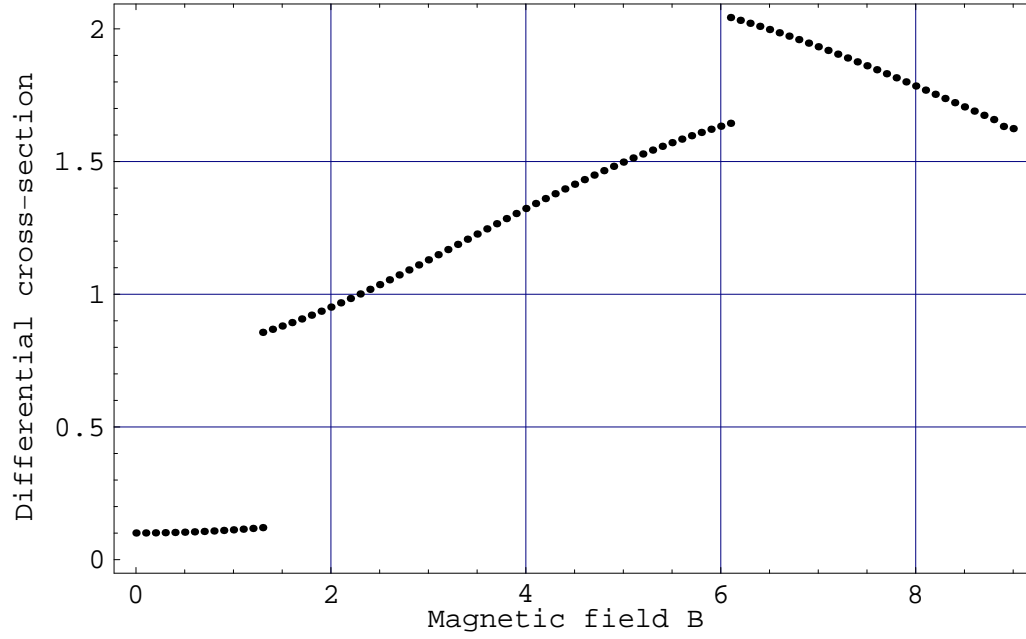
Figure 5: $\frac{\frac{d\sigma}{d\phi_{\vec{q}}}}{\sigma_0}$ vs. B(T) is plotted for different 'm' values of the ground state as the B is varied and showing discontinuities as characteristic of the transitions. From the plot it is found that percentage change for $m = 1 \rightarrow m = 2$ is $\approx 4.5$ times smaller compared to $m = 0 \rightarrow m = 1$ transition and also it is evident from the plot that at a fixed frequency behaviors of different 'm' cross-sections are going to change and for this reason both $\omega$ and B have to be varied to observe all the transitions properly.